

## Supporting Information

### Regulating the synthesis rate and yield of bio-assembled FeS nanoparticles for efficient cancer therapy

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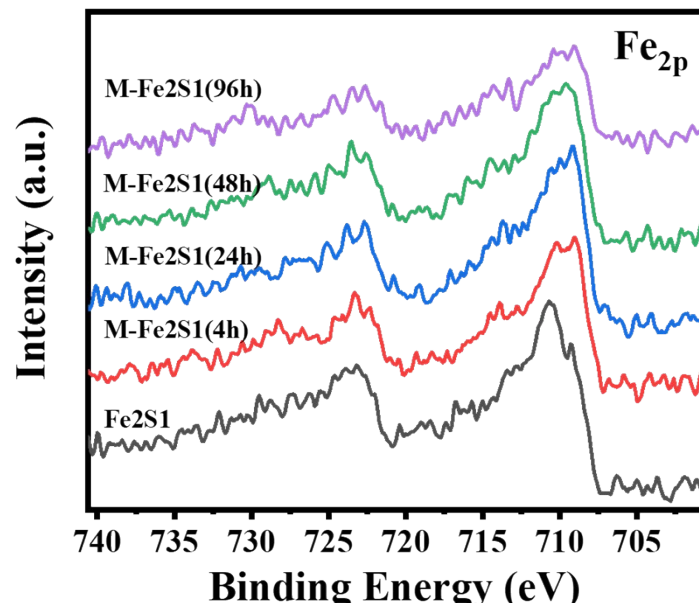
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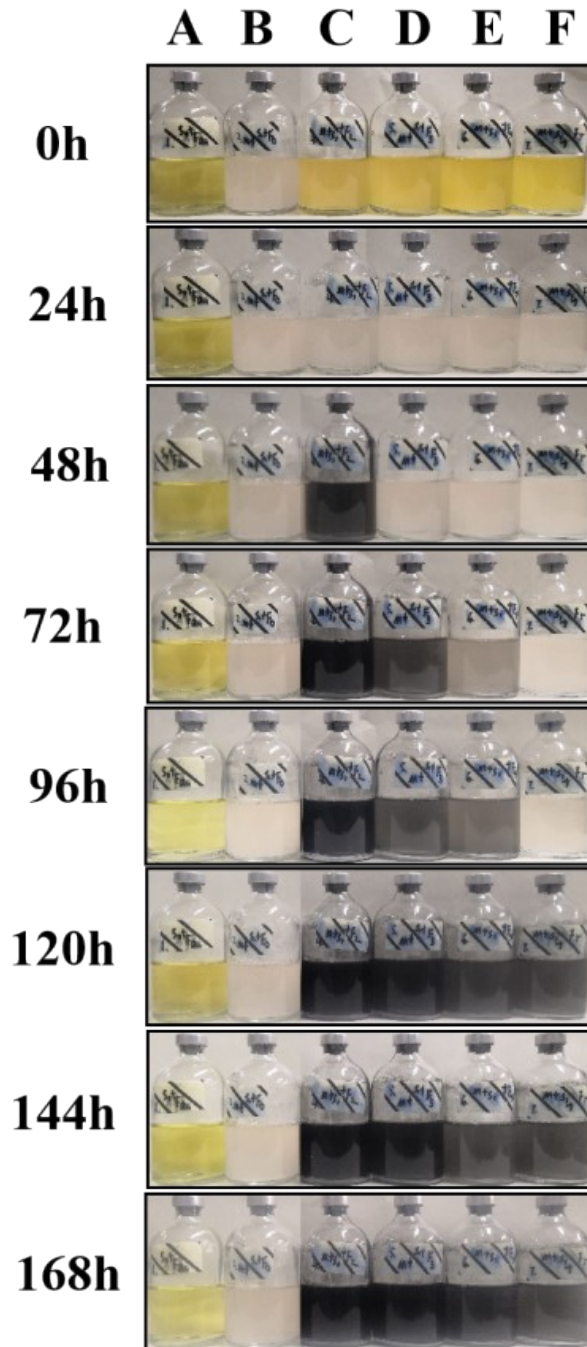
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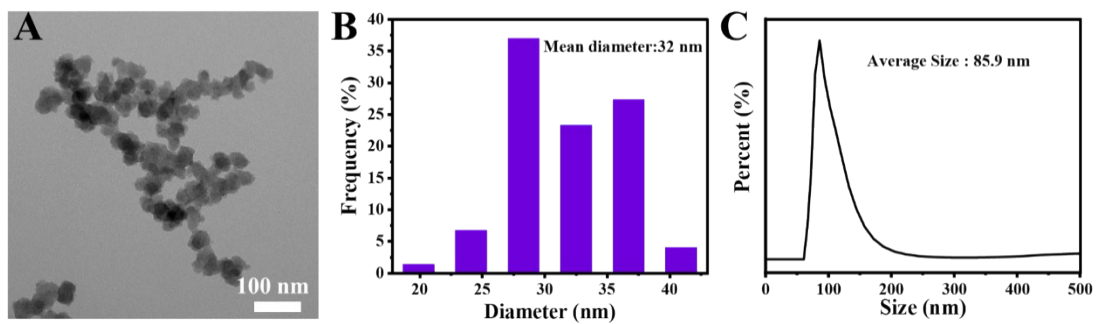
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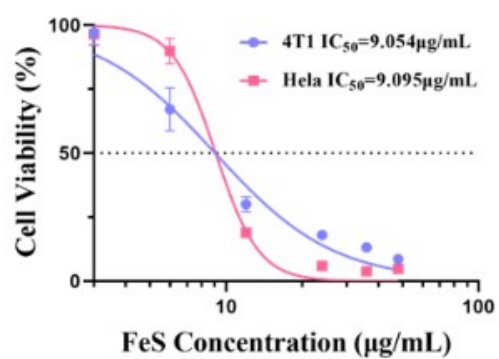
**Fig. S1.** Time-resolved Fe 2p XPS patterns of the biogenic system. Fe2 refers to 2 mM Fe(III)-citrate. S1 refers to 1 mM thiosulfate. M refers to *S. oneidensis* MR-1.



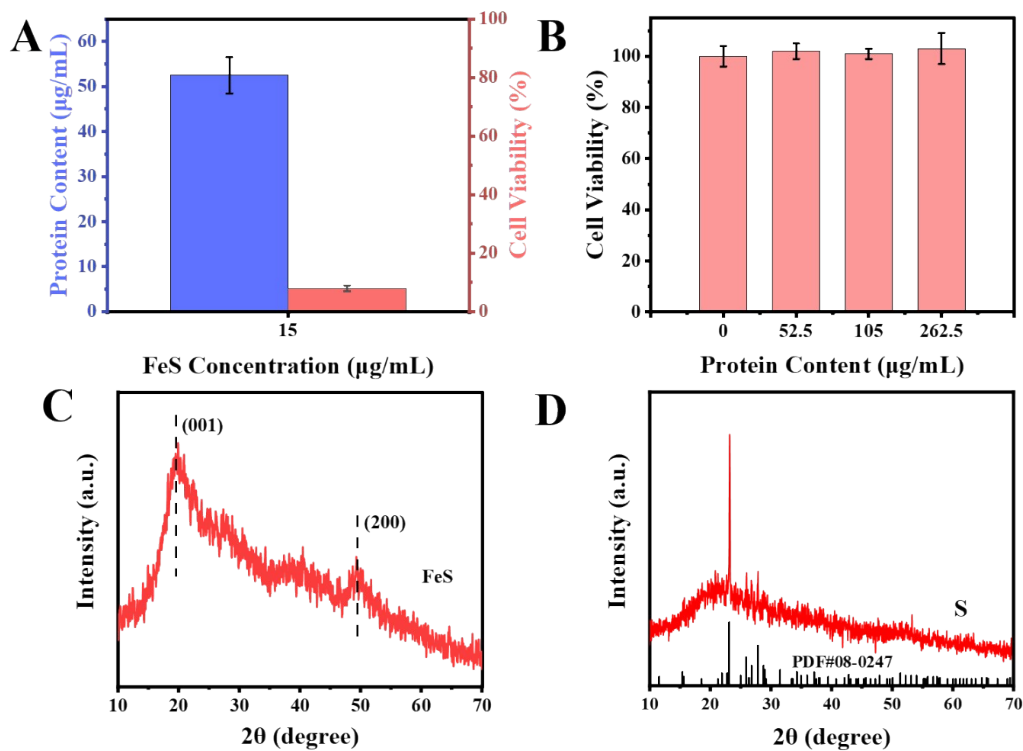
**Fig. S2.** Images of *S. oneidensis* MR-1 cells suspension collected at different incubation times under bright field. Cells were cultivated with 1mM thiosulfate and different Fe(III)-citrate contents. **A** refers to Fe2S1 group, **B** refers to M-S1 group, **C** refers to M-Fe2S1 group, **D** refers to M-Fe3S1 group, **E** refers to M-Fe4S1 group, **F** refers to M-Fe5S1 group.



**Fig. S3.** The characteristics of the purified FeS NPs. (A) The TEM image of Bio-FeS NPs. (B) Size distribution of the Bio-FeS NPs calculated from TEM image.(C) The DLS size distribution of the purified Bio-FeS NPs in water.



**Fig. S4.** Half inhibitory concentration (denoted as IC<sub>50</sub>) of Bio-FeS NPs were calculated using GraphPad Prism software (version 6.01)



**Fig. S5.** The functions of proteins capped on FeS NPs. (A) Protein content and cell viability of 15  $\mu\text{g/mL}$  FeS nanoparticles. (B) Cell viabilities of HeLa cells after being treated with different concentrations of proteins extracted from bacteria. XRD spectrums of protease K (C) untreated and (D) treated Bio-FeS NPs.

**Table S1.** Evaluation of the Fenton (Fenton-like) agents therapy efficiency.

| Materials  | Cell line | Content ( $\mu\text{g/mL}$ ) | Incubation time(h) | Survivals (~%) | Ref. |
|--|-----------|------------------------------|--------------------|----------------|------|
| One-Dimensional Fe <sub>2</sub> P (NRs)  | Hela      | 25                           | 24                 | 98             | 1    |
|  |           | 50                           |                    | 95             |      |
|  |           | 100                          |                    | 91             |      |
|  |           | 200                          |                    | 90             |      |
|  |           | 300                          |                    | 85             |      |
| mesoporous copper/manganese silicate nanospheres (mCMSNs)                          | MCF-7     | 1                            | 24                 | 95             | 2    |
|  |           | 5                            |                    | 91             |      |
|  |           | 10                           |                    | 85             |      |
|  |           | 20                           |                    | 56             |      |
|  |           | 50                           |                    | 30             |      |
|  |           | 100                          |                    | 23             |      |
| 200  | 21        |                              |                    |                |      |
| MnO <sub>2</sub> -coated mesoporous silica nanoparticles (MS@MnO <sub>2</sub> NPs) | U87MG     | 1                            | 24                 | 91             | 3    |
|  |           | 2                            |                    | 80             |      |
|  |           | 5                            |                    | 62             |      |
|  |           | 10                           |                    | 52             |      |
|  |           | 20                           |                    | 38             |      |
| Cu/CC NPs  | A549      | 25                           | 24                 | 92             | 4    |
|  |           | 50                           |                    | 79             |      |
|  |           | 100                          |                    | 66             |      |
|  |           | 150                          |                    | 60             |      |
|  |           | 200                          |                    | 51             |      |
|  | 4T1       | 25                           | 24                 | 75             |      |
|  |           | 50                           |                    | 71             |      |
|  |           | 100                          |                    | 68             |      |
|  |           | 150                          |                    | 56             |      |
|  |           | 200                          |                    | 38             |      |
| DSF@PEG/Cu-HMSNs   | 4T1       | 0.6                          | 24                 | 94             | 5    |
|  |           | 1.25                         |                    | 92             |      |
|  |           | 2.5                          |                    | 80             |      |
|  |           | 5                            |                    | 52             |      |
|  |           | 10                           |                    | 30             |      |
|  |           | 20                           |                    | 12             |      |
| Cu-HCF single-site nanozymes (SSNEs)   | Hela      | 12.5                         | 24                 | 100            | 6    |
|  |           | 25                           |                    | 80             |      |
|  |           | 50                           |                    | 60             |      |
|  |           | 100                          |                    | 48             |      |
|  |           | 200                          |                    | 30             |      |

|  |             |   |           |  |    |
|--|-------------|---|-----------|--|----|
| Cu-HCF single-site nanozymes (SSNEs)   | 4T1         | 12.5<br>25<br>50<br>100<br>200                      | 24        | 98<br>75<br>65<br>53<br>25                   | 6  |
| iron-containing metal-organic framework [MOF(Fe)] nanocatalyst   | Hela        | 2<br>4<br>8<br>16<br>32<br>64                       | 24        | 99<br>95<br>90<br>85<br>78<br>70             | 7  |
| (FeS@BSA) nanoclusters   | Huh7        | 4<br>8<br>12<br>16<br>20                            | 24        | 98<br>80<br>32<br>22<br>20                   | 8  |
| core-shell-structured iron carbide (Fe <sub>5</sub> C <sub>2</sub> @Fe <sub>3</sub> O <sub>4</sub> ) nanoparticles (NPs) | 4T1         | 50<br>100<br>150<br>200<br>250<br>300<br>350<br>400 | 24        | 98<br>94<br>92<br>91<br>87<br>71<br>63<br>57 | 9  |
| FeGd-HN@Pt@LF/RGD2   | MCF-7       | 1.75<br>3.5<br>7<br>14<br>28<br>56                  | 24        | 94<br>99<br>92<br>90<br>81<br>75             | 10 |
|  | U-87        | 1.75<br>3.5<br>7<br>14<br>28<br>56                  | 24        | 66<br>50<br>41<br>39<br>28<br>24             | 10 |
| <b>Bio-FeS NPs</b>   | <b>Hela</b> | <b>3<br/>6<br/>12<br/>24<br/>36<br/>48</b>          | <b>24</b> | <b>98<br/>90<br/>19<br/>6<br/>5<br/>6</b>    |    |



|                    |            |           |           |            |  |
|--------------------|------------|-----------|-----------|------------|--|
| <b>Bio-FeS NPs</b> | <b>4T1</b> | <b>3</b>  | <b>24</b> | <b>100</b> |  |
|                    |            | <b>6</b>  |           | <b>65</b>  |  |
|                    |            | <b>12</b> |           | <b>30</b>  |  |
|                    |            | <b>24</b> |           | <b>19</b>  |  |
|                    |            | <b>36</b> |           | <b>12</b>  |  |
|                    |            | <b>48</b> |           | <b>8</b>   |  |

**Table S2** The employed bacteria for FeS NPs biosynthesis

| Species                       | NPs              | S-source                                      | Fe-source         | Size (nm)       | Applications               | Ref.      |
|-------------------------------|------------------|---|-------------------|-----------------|----------------------------|-----------|
| <i>S. oneidensis</i> MR-1     | FeS              | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> | FeCl <sub>3</sub> | 30              | microbial fuel cells (MFC) | 11        |
| <i>S. oneidensis</i> MR-1     | FeS              | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> | Fe-citrate        | 60              | microbial electrochemical  | 12        |
| <i>A. cryptum</i> JF-5&SRB    | FeS              | SO <sub>4</sub> <sup>2-</sup>                 | FeSO <sub>4</sub> | -               | remediation                | 13        |
| <i>Desulfovibrio vulgaris</i> | FeS              | NaSO <sub>4</sub> , MgSO <sub>4</sub>         | FeSO <sub>4</sub> | several to tens | -                          | 14        |
| <i>S. oneidensis</i> MR-1     | FeS              | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> | naphthol green B  | 30              | contaminant degradation    | 15        |
| <i>S. putrefaciens</i> CN32   | FeS              | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> | Fe-citrate        | 100             | contaminant degradation    | 16        |
| <i>Shewanella</i> PV-4        | FeS              | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> | FeCl <sub>3</sub> | 5-10            | MFC                        | 17        |
| <i>Geobacter</i>              | FeS <sub>2</sub> | (NH <sub>2</sub> ) <sub>2</sub> CS            | FeCl <sub>3</sub> | 26-48           | MFC                        | 18        |
| <i>S. oneidensis</i> MR-1     | FeS              | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> | Fe-citrate        | 35              | biomedicine                | This work |

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